RESEARCH OF THE FORMATION POSSIBILITY OF THE NANORESONATOR BASED ON 2D-H-BN SURFACE

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Abstract. In microworld some materials with adsorbed metal atoms on their surface can act as a resonators in case the metal atoms are considered as conductive lines. In this paper we have studied the possibility of 2D-h-BN modification by lithium atoms to use this new 2D material as base of a nanoresonator in the future.

After the revolutionary discovery of graphen [1], the research interest of the new materials which can be considered as a two-dimensional structures has been rapidly increased.

It is expected that two-dimensional materials will be effectively used as functional blocks and devices of new generation nanoelectronics. They will find an application in power engineering and optics, and in the synthesis of new structural and composite materials based on it. In 2015 two-dimensional boron nitride was successfully synthesized and has been started actively studied by many scientific communities since then [2]. Boron nitride (h-BN) is an isoelectronic and an isostructural analogue of graphite and now it is a member of the 2D nanostructure family. Graphen-like h-BN can be used for creation of hyperbolic metasurfaces as had been shown in the research of the scientists group of Rainer Hillenbrand from Spain and USA [3]

The first step of our research was the investigation of the binding opportunity between the atom of lithium or natrium and the surface of 2D-h-BN and the mechanism of this process. Due to the locality of the problem, the calculations were carried out within the model of molecular cluster of h-BN sheet with the use of quantum chemical MNDO scheme [4].

The calculations have allowed to model profiles of potential energy surface of the given processes. The energy curves of these processes show a minimum (excluding the case with atom Na over the atoms of a surface) which illustrates the fact of a chemical bond formation between Li atoms and atoms on the surface of 2D-h-BN. A Na atom is not adsorbed over the atoms of the 2D-h-BN surface. The analysis of adsorption energy values showed that the best location for Li is over an atom N, the potential energy well is deeper.

The adsorption possibility of lithium by 2D-h-BN surface allowed us to study the regular adsorption of group of atoms Li. So, groups of 11, 16 and 21 lithium atoms (lithium chain) have been arranged in a certain way over the h-BN surface at a distance of 2.2 Å (distance of atomic adsorption), as you can see on the figure 1. To assess the stability of lithium chains, we have calculated the value of the total energy of the same structures, but with some chains modification. One of the Li atom has been located out

of the lithium chain. The difference of total energies of these structures is around 0,05 eV, and the open rings in which all lithium atoms have located one after another (without break) are energetically more stable and therefore the 2D-h-BN structures with lithium modification on the surface as have shown in figure 1 are presumable and can be use as base for nanoresonators. This fact gives an additional capability for creation a new metamaterials which can be work on ultra short wave-length.

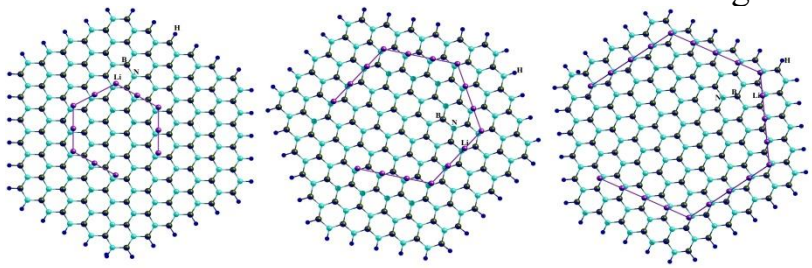

Fig. 1. 2D-h-BN with the lithium chain over the surface: a) 11Li; b) 16Li; c) 21 Li

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